Title: COMPUTER-AIDED OPTIMIZATION OF SUBSTANCE LIBRARIES
Inventor(s): Dr. Stephen A. SCHUNK
Dr. John M. NEWSAM
DOCKET NO.: 078096/0105
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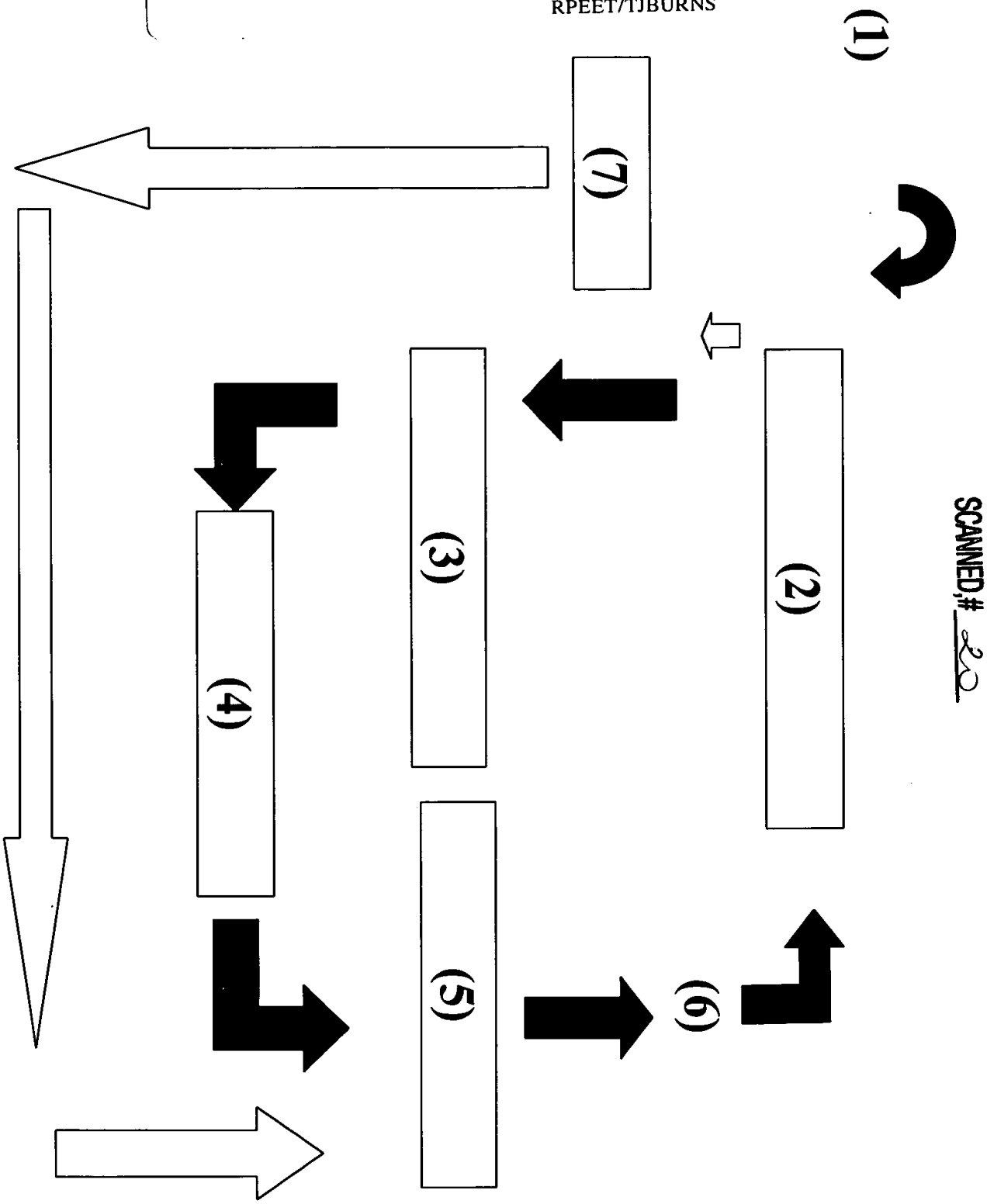

Fig. 1

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Performance Characteristics

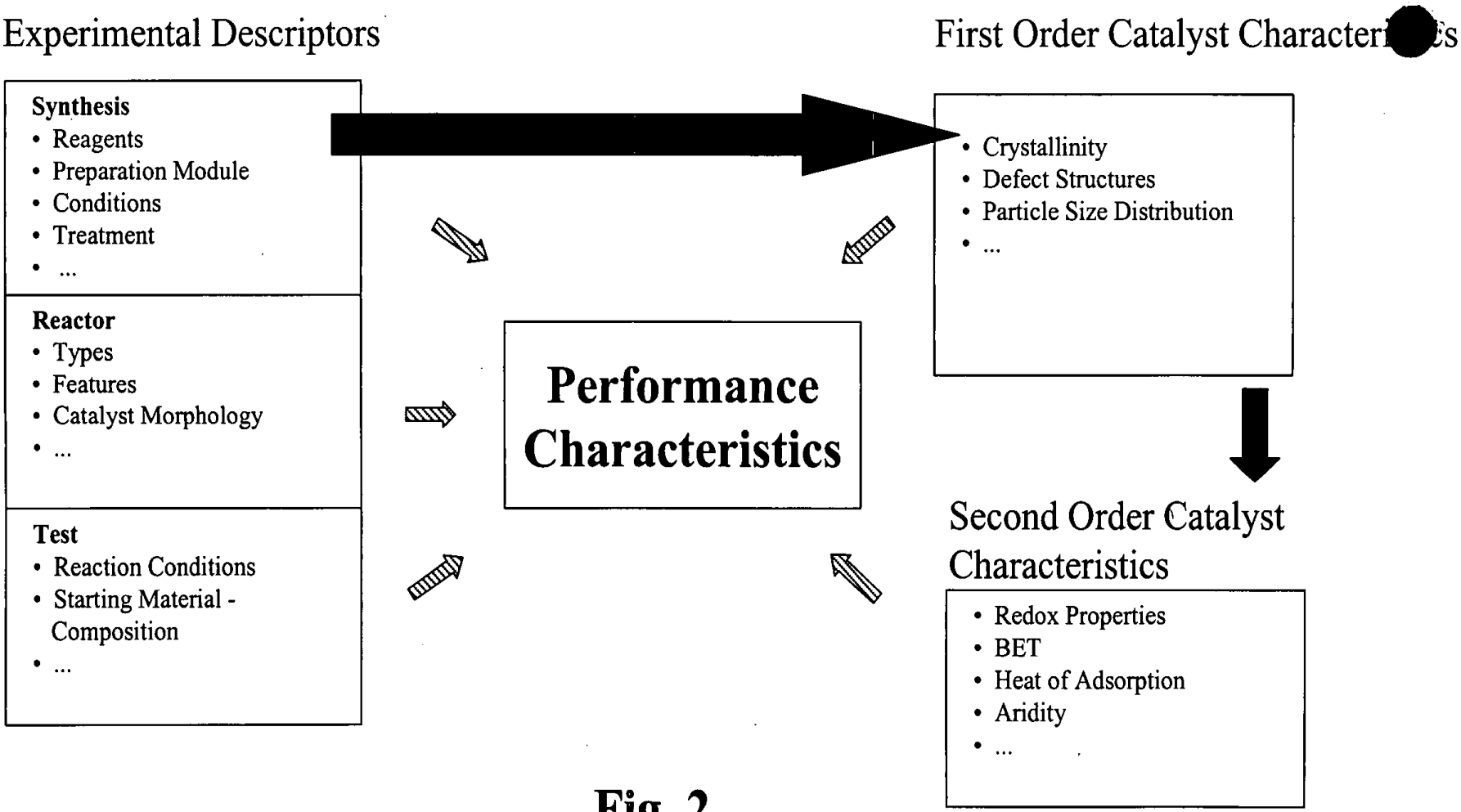

Fig. 2

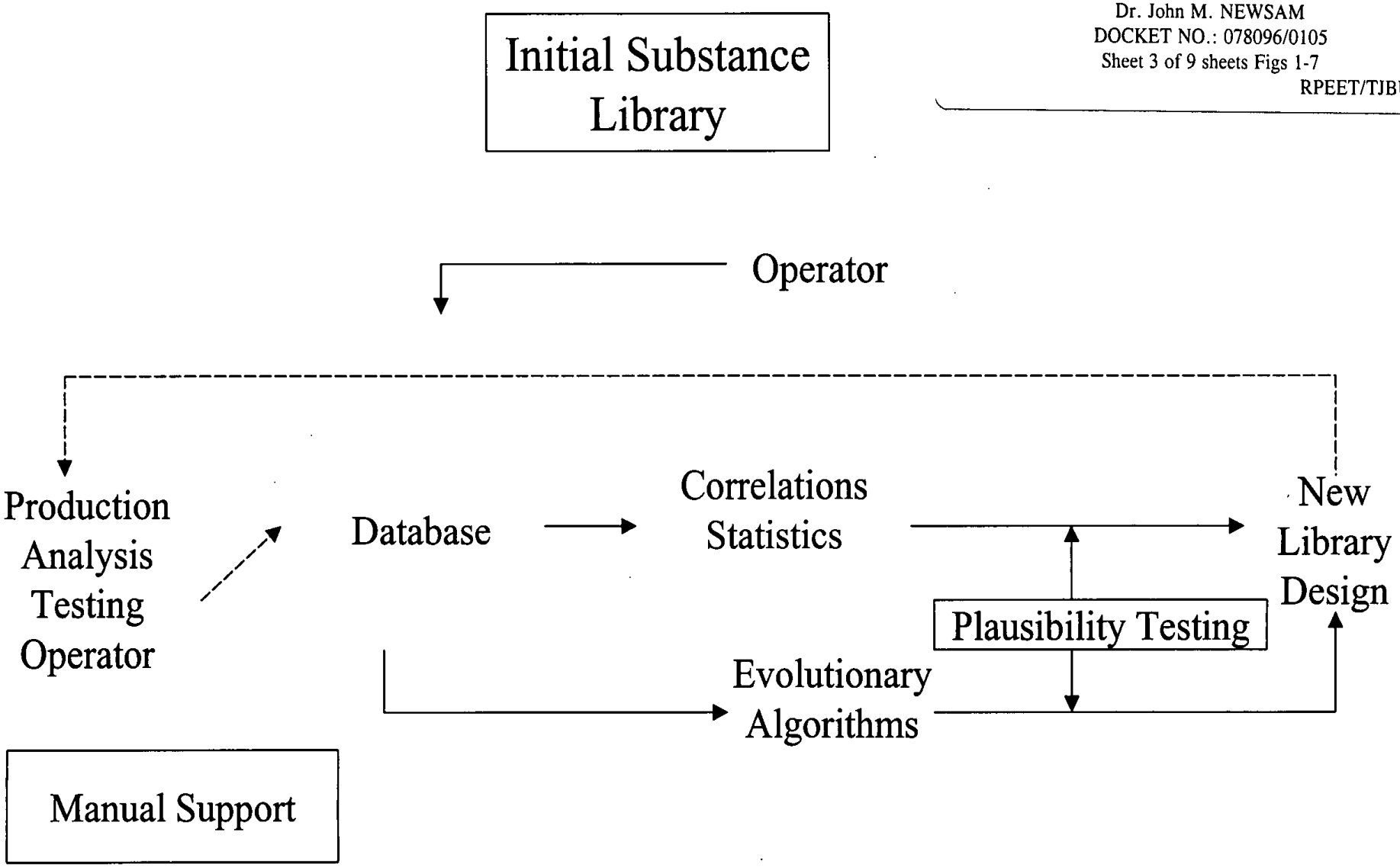
Initial Substance Library
Operator
Production Analysis Testing Operator
Database
Correlations Statistics
New Library Design
Plausibility Testing
Evolutionary Algorithms
Manual Support

Fig. 3

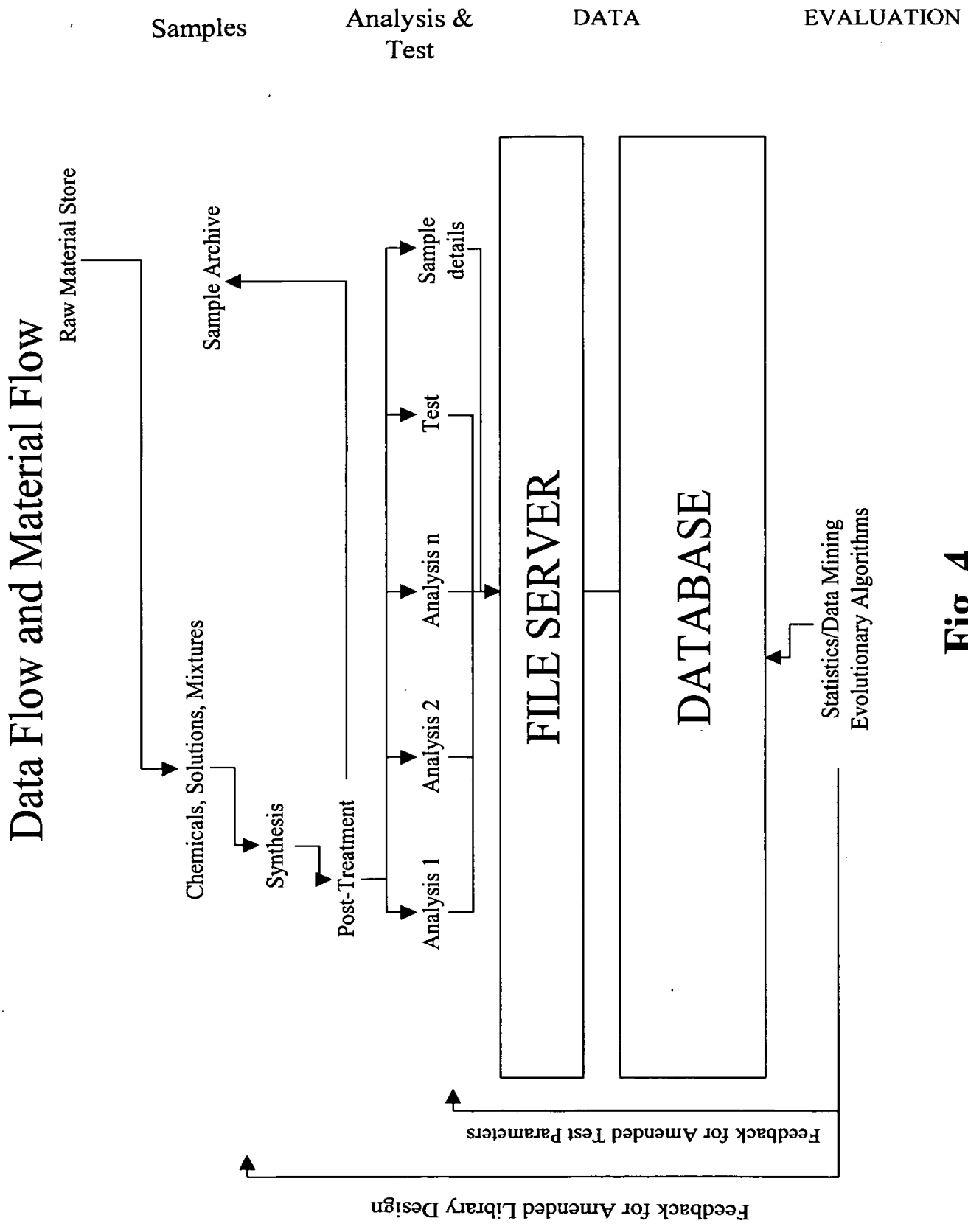
Samples
Analysis & Test
DATA
EVALUATION
Data Flow and Material Flow
Raw Material Store
Sample Archive
Sample details
Chemicals, Solutions, Mixtures
Synthesis
Post-Treatment
Analysis 1
Analysis 2
Analysis n
Test
FILE SERVER
DATABASE
Statistics/Data Mining
Evolutionary Algorithms
Feedback for Amended Test Parameters
Feedback for Amended Library Design

Fig. 4

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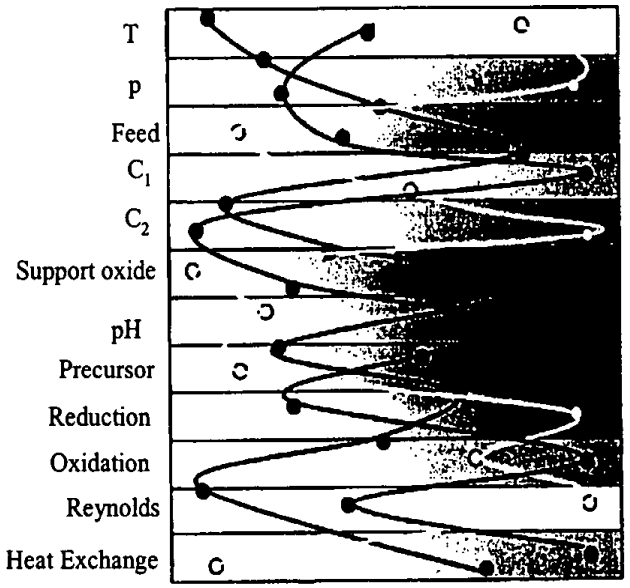
Original Library Design and Tests Using the Entire Parameter Space

Step 1: Design of Library, Test and Process Conditions



Step 2: Data Acquisition

	Experiment 1	Experiment 2	Experiment n
T			
p			
Feed			
C_1			
C_2			
Support oxide			
PH			
Precursor			
Reduction			
Oxidation			
Reynolds			
Heat Exchange			

Activity	++	+	+++
Selectivity	+	++	–

Fig. 5a

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Regression Analysis, Energies of the Parameter Space

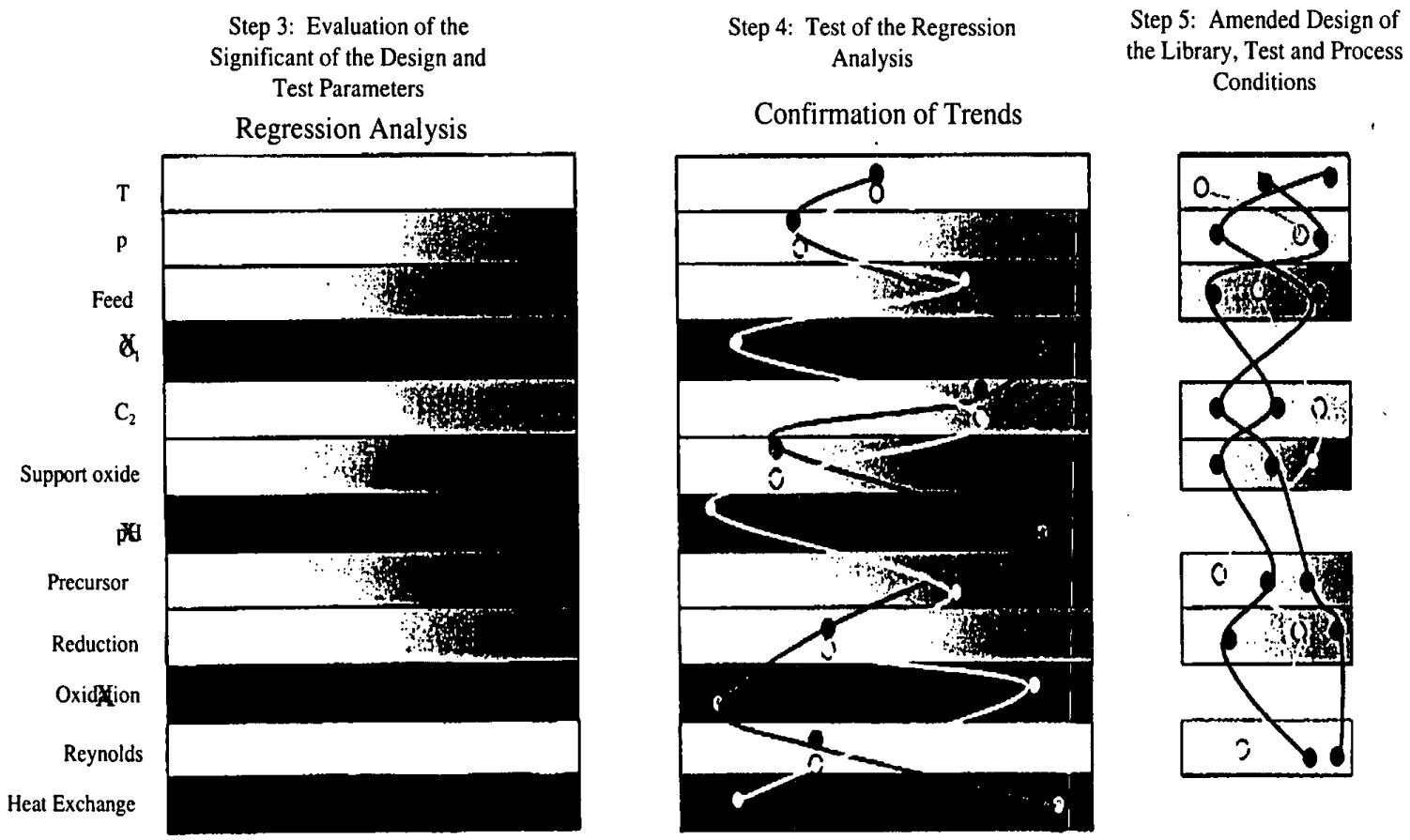

Fig. 5b

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Principle of Genetic Algorithms

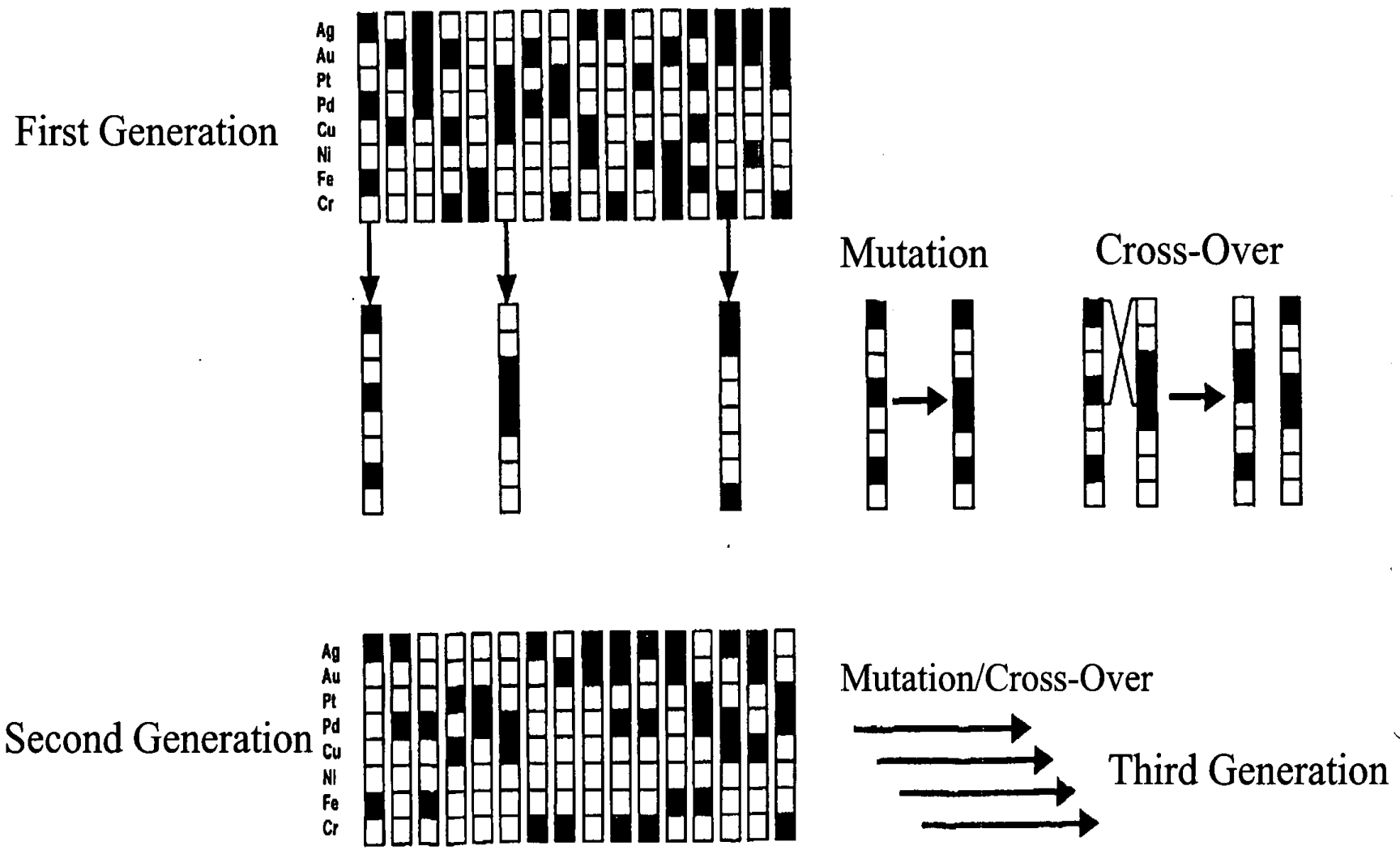

Fig. 5c

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Sensitivity Analysis of the Parameters of the Initial Library Pareto Diagram

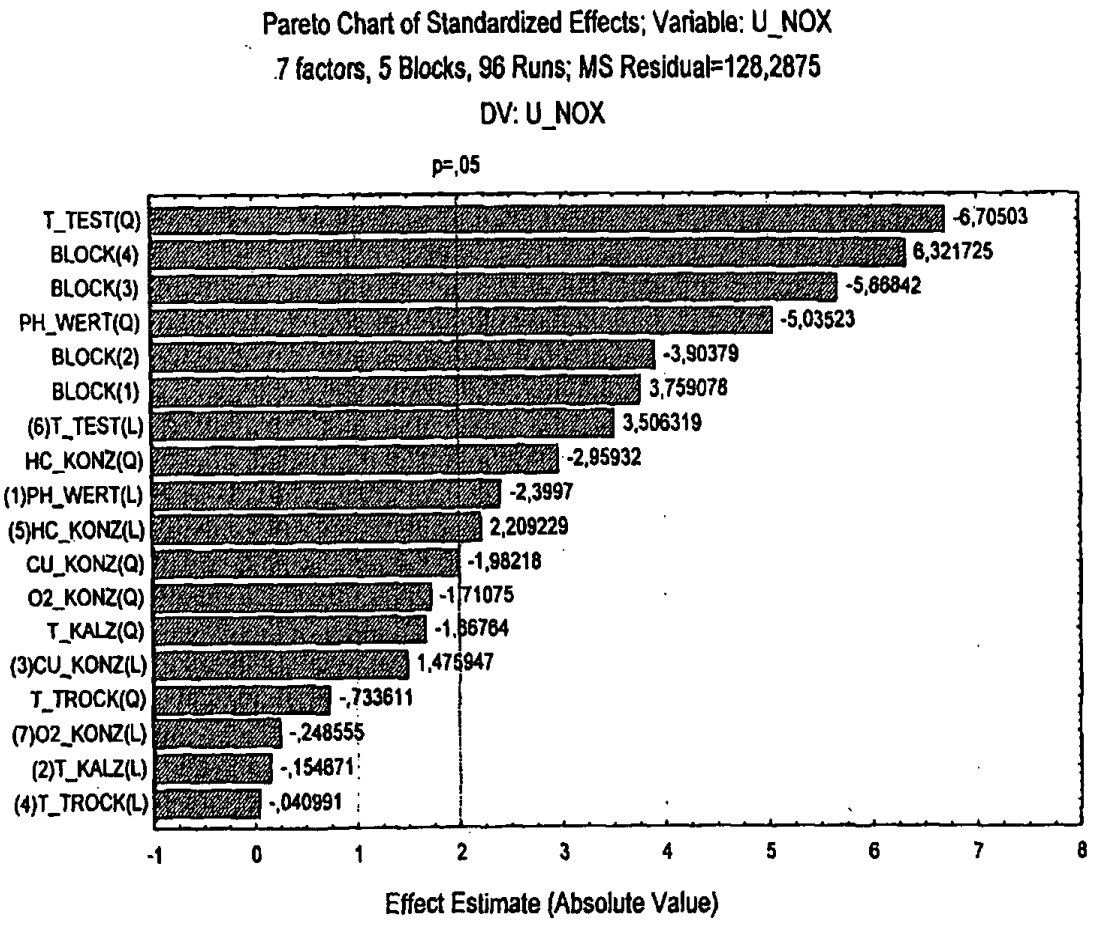

Fig. 6

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Sensitivity Analysis of the Parameters of the 1st Optimized Library Pareto Diagram

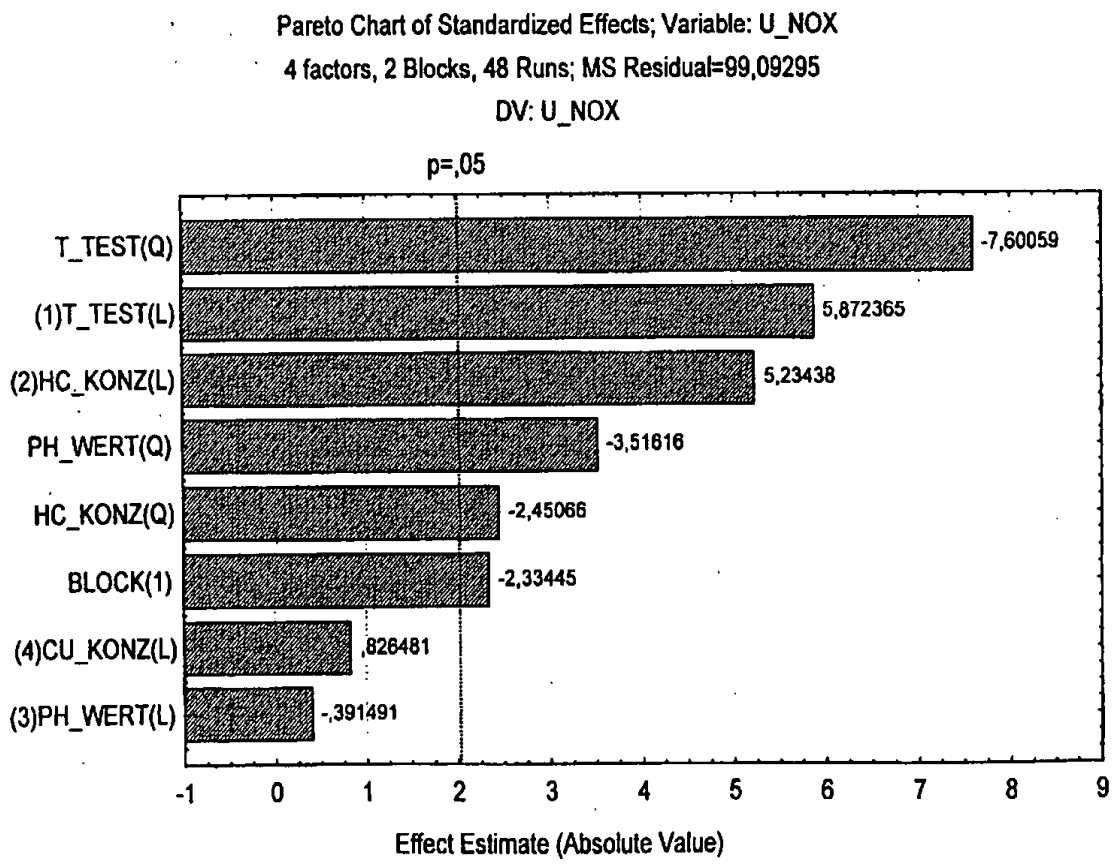

Fig. 7

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